On the excluded space in applications of Feshbach projection formalism

S. Karataglidis*

Department of Physics and Electronics, Rhodes University,
P.O. Box 94, Grahamstown, 6140, South Africa.

K. Amos†

School of Physics, University of Melbourne, Victoria 3010, Australia

(Dated: February 2, 2008)

Abstract

Various model applications in nuclear structure and reactions have been formulated starting with the Feshbach projection formalism. In recent studies a truncated excluded space has been enumerated to facilitate calculation and identify a convergence in expansions within that truncation. However, the effect of any remainder must be addressed before results from such can be considered physical.

PACS numbers:

*Electronic address: S.Karataglidis@ru.ac.za
†Electronic address: amos@physics.unimelb.edu.au

Interest in the Feshbach projection formalism as a way to unify reaction and structure theory has increased in recent years with studies such as those of the no-core shell model (SM), like those made using G-matrix interactions [1], and of the continuum shell model [2]. With reaction theory, the formalism lies at the heart of the recent multi-channel algebraic scattering (MCAS) theory [3] though applications of that method [4] so far assume that all important channels have been included in the $\mathcal{P}$ space. However, the formalism has long been used to make the framework of the optical model for elastic scattering [5, 6]. In that use, all channels other than those of the elastic scattering are taken to form the excluded space $\mathcal{Q}$ while the elastic channels span the space supposedly treated exactly. The dual space formalism is elegant but it is almost totally impractical due to the (usually large) number of reaction channels to be considered in defining terms such as the dynamic polarization potential. Often then, either a total phenomenological approach or a restricted selection of terms of importance in the excluded space need be made to facilitate evaluations. While the foregoing centered on reaction theory, such is also the case when the formalism is applied to consider properties of an isolated nucleus as with the G-matrix SM of Navrátil and Barrett [1] and with the Continuum Shell Model (CSM) of Volya and Zelelevinsky [2]. The question arises as to the convergence of solutions obtained in the truncated ($\mathcal{Q}$) space to those of the actual complete space.

The dual space form of the Feshbach theory [5, 6] fragments the Hilbert space $\{\Psi\}$ into subspaces $\mathcal{P}$ and $\mathcal{Q}$ by the action of projection operators P and Q respectively on the space spanned by the eigenfunctions Ψ of the full Hamiltonian. The subspace $\mathcal{P}$ is spanned by the functions $P\Psi$ while that of $\mathcal{Q}$ is spanned by $Q\Psi$. The assumption is that the solutions within P space can be evaluated while that of the full space $\mathcal{P} + \mathcal{Q}$ cannot. As projection operators, P and Q satisfy the conditions

$$\begin{aligned} P^2 = P; \qquad Q^2 = Q; \qquad PQ = QP = 0 \\ P + Q = 1. \end{aligned} \tag{1}$$

Then, with the notation $H_{XY} = XHY$, where X, Y are any combination of the operators P, Q, the complete Schrödinger equation can be recast as

$$\begin{aligned} (E - H_{PP})\, P\Psi &= H_{PQ} Q\Psi \\ (E - H_{QQ})\, Q\Psi &= H_{QP} P\Psi. \end{aligned} \tag{2}$$

Using the second of these to define $Q\Psi$ in terms of $P\Psi$ then defines the $\mathcal{P}$ space equation to be solved, namely

$$\left[E - H_{PP} - H_{PQ} \frac{1}{(E - H_{QQ})} H_{QP} \right] P\Psi = 0. \tag{3}$$

Thus the contribution to the full Hamiltonian from coupling to the excluded states (the so-called "doorway" states) is defined as the additional term

$$\Delta H = H_{PQ} \frac{1}{(E - H_{QQ})} H_{QP}. \tag{4}$$

If one restricts consideration first to nucleon-nucleus (NA) scattering, where the $\mathcal{P}$ space may be taken to define only elastic scattering, then ΔH is the dynamic polarization potential aspect of the optical potential. It is an energy-dependent problem to evaluate. At

low energies, as evidenced by MCAS studies [7], and for light masses particularly, channel coupling of the nucleon to excited states of the target are the essential elements. The DPP that results is highly non-local, complex, and energy- and angular momentum dependent. One consequence is that phenomenological local potentials which are often used are not physically justified. For such cases it seems that the $\mathcal{Q}$ space may be enumerated with coupling of the incident nucleon to relatively few states of the target nucleus. At higher incident energies, values for which the giant resonances of the target may be excited, past studies have noted their influence in scattering as doorway states in second order processes [8]. Other channels which reflect in those studies require residual complex (phenomenological) optical potentials; they should be nonlocal. When the available energy coincides with the target in its continuum, a successful way to enumerate $\mathcal{Q}$ space effects is to adapt the KMT theory [9]. That has been done, for example, with the so-called g-folding optical potential [10]. For those energies, one cannot enumerate $\mathcal{Q}$ space in any detail but its effects in many applications to date [10, 11] seem encompassed in the medium and Pauli blocking effects defined in the infinite matter g-matrices upon which the g-folding model is based.

A truncated Hilbert space is also the key feature of the shell model for nuclear structure; being essential for practical calculation. One may define the $\mathcal{P}$ space as that in which the SM interaction is defined. The $\mathcal{Q}$ space then encompasses all of the higher $\hbar\omega$ admixtures lying outside and which can have effects due to long range correlations. It is well known that by restricting the $\mathcal{P}$ space to be just the $0\hbar\omega$ for valence nucleons requires polarization charges, typically of $0.5e$, to match the associated model results to observation. Such is a reflection of higher $\hbar\omega$ correlations. However, by increasing the basis size, e.g. to encompass a complete $(0+2)\hbar\omega$ space, then there remain yet higher order correlations that may still play an important role. Whatever the space enlargement with a SM, one still has missing pieces by definition.

The G-matrix SM model interaction of Navrátil and Barrett [1] as used later [12, 13, 14], considers coupling up to three-body correlations. In that no-core SM, the $\mathcal{Q}$ space is assumed to be made of states including only those 2- and 3-body correlations above those included in the $\mathcal{P}$ space. However, then $P + Q \neq 1$ by construction. Higher order correlations may become important as the mass of the nucleus increases, and with them, the probability of forming large clusters. ^{12}C is a case in point. First there is the success of the α-cluster model in explaining the super-deformed 0^+ state at 7.6 MeV, which suggests 4-particle correlations at least must be included in the SM. Second, it was observed that the excitation energy of the 2_1^+ state diverged from the experimental value as the model space was increased. Finally the predicted $B(E2; 2_1^+ \to 0_1^+)$ is not in good enough agreement with the measured value. Even including a three nucleon force, as was done recently [14], did not make much improvement. By contrast, when using the (fitted) MK3W interaction in the $(0+2)\hbar\omega$ model space, very good results for the spectrum and for the electron scattering form factors were found for ^{12}C [15]. The action of the fitting in determining the interaction implicitly includes higher-order correlations not considered in the those *ab initio* interactions. While the fitted interactions are not *ab initio*, the use of them does illustrate the effect of the $\mathcal{Q}$ space.

The CSM calculations [2] allow coupling to the continuum via one- and two-particle excitations. They consider the effects of coupling to the continuum (their restricted $\mathcal{Q}$ space) above the standard shell model ($\mathcal{P}$ space). By so doing they ascribe widths to resonance states without changing the energy of that state from what was found from a $\mathcal{P}$ space calculation. However, coupling to the $\mathcal{Q}$ space necessarily requires that there be

contributions from such coupling also to the real part of energy eigenvalues. The effects of higher order correlations remains also unknown for this model.

To consider such limitations made upon the actual $\mathcal{Q}$ space of any problem, we make a three space development of the Feshbach formalism. The Hilbert space is divided now into the $\mathcal{P}$, a reduced, enumerable, $\mathcal{Q}$, and a new remainder $\mathcal{R}$ spaces. There are three associated projection operators, P, Q, and R satisfying $P + Q + R = 1$. In this case the Schrödinger equation can be cast into the three projected, coupled equations

$$\begin{aligned}(E - H_{PP})\, P\Psi &= (H_{PQ}Q\Psi + H_{PR}R\Psi) \\ (E - H_{QQ})\, Q\Psi &= (H_{QP}P\Psi + H_{QR}R\Psi) \\ (E - H_{RR})\, R\Psi &= (H_{RP}P\Psi + H_{RQ}Q\Psi)\,. \end{aligned} \tag{5}$$

These equations reduce to those of Eq. (2) in the limit that couplings to $\mathcal{R}$ space can be neglected. Such seem to be the case for NA scattering at low and intermediate energies. Rearranging Eqs. (5) gives

$$\begin{aligned} Q\Psi &= \frac{1}{(E - H_{QQ})}\left[H_{QP}P\Psi + H_{QR}R\Psi\right] \\ R\Psi &= \frac{1}{(E - H_{RR})}\left[H_{RP}P\Psi + H_{RQ}Q\Psi\right]. \end{aligned} \tag{6}$$

Using the second equation for $R\Psi$ in the first, and rearranging, gives

$$Q\Psi = \left[1 - \frac{1}{(E - H_{QQ})}H_{QR}\frac{1}{(E - H_{RR})}H_{RQ}\right]^{-1} \frac{1}{(E - H_{QQ})}\left[H_{QP} + H_{QR}\frac{1}{(E - H_{RR})}H_{RP}\right]P\Psi. \tag{7}$$

Likewise one can eliminate $Q\Psi$ from the Eqs. (6) and rearrange the result to find

$$R\Psi = \left[1 - \frac{1}{(E - H_{RR})}H_{RQ}\frac{1}{(E - H_{QQ})}H_{QR}\right]^{-1} \frac{1}{(E - H_{RR})}\left[H_{RP} + H_{RQ}\frac{1}{(E - H_{QQ})}H_{QP}\right]P\Psi. \tag{8}$$

Then substituting Eqs. (7) and (8) into the first of Eqs. (5) gives the $\mathcal{P}$ space equations

$$\begin{aligned} \Bigg\{ E - H_{PP} - H_{PQ}&\left[1 - \frac{1}{(E - H_{QQ})}H_{QR}\frac{1}{(E - H_{RR})}H_{RQ}\right]^{-1} \\ &\frac{1}{(E - H_{QQ})}\left[H_{QP} + H_{QR}\frac{1}{(E - H_{RR})}H_{RP}\right] \\ &- H_{PR}\left[1 - \frac{1}{(E - H_{RR})}H_{RQ}\frac{1}{(E - H_{QQ})}H_{QR}\right]^{-1} \\ &\frac{1}{(E - H_{RR})}\left[H_{RP} + H_{RQ}\frac{1}{(E - H_{QQ})}H_{QP}\right]\Bigg\} P\Psi = 0. \end{aligned} \tag{9}$$

Again for situations where coupling to $\mathcal{R}$ space can be ignored, $(H_{PR} = H_{QR} = 0)$, this reduces to the form given in Eq. (2). If expansion is restricted to third order in couplings, each inverse bracket term in Eq. (9) becomes the unit operator so that a reduced $\mathcal{P}$ space equation is

$$\Big\{E - H_{PP} - H_{PQ}\frac{1}{(E - H_{QQ})}H_{QP} - H_{PR}\frac{1}{(E - H_{RR})}H_{RP} - H_{PQ}\frac{1}{(E - H_{QQ})}H_{QR}\frac{1}{(E - H_{RR})}H_{RP} - H_{PR}\frac{1}{(E - H_{RR})}H_{RQ}\frac{1}{(E - H_{QQ})}H_{QP}\Big\} P\Psi = 0. \quad (10)$$

Thus the coupling to excluded space of a problem may be via coupling to either the $\mathcal{Q}$ or $\mathcal{R}$ subspaces at second order in the expansion as well as via the chains $\mathcal{P} \to \mathcal{Q}(\mathcal{R}) \to \mathcal{R}(\mathcal{Q}) \to \mathcal{P}$ in third order. The states in $\mathcal{R}$ space more than play the role of hallway states in past studies, for we now allow for states therein that directly connect by couplings omitted in the enumerated $\mathcal{Q}$ space. To the extent that coupling to those states in $\mathcal{R}$ space is not negligible, such have effect even at second order in expansions. Thus, unless one can ensure all important couplings are collected within an enumerated $\mathcal{Q}$ space, then no matter how much, and to what order, the effects of the enumerated $\mathcal{Q}$ space are taken, errors arise at the second order level. Results of using the G-matrix interaction developed by Navrátil and Barrett [1] in large space no-core shell model calculations for systems (such as ^{6}Li [16] and ^{12}C [13, 14]) which exhibit features of α-clustering, and so of four-body correlations, give evidence of such omission. That approach does show convergence to the enumerated $\mathcal{Q}$ space complete values, but those values remain far from the empirical ones. The problem starts at second order. Indeed, neglect of the higher order correlations in that G-matrix interaction has already been identified as a potential problem [16]. In contrast, the earlier interactions developed by Zheng *et al.* [17] seem to accommodate such higher order effects through the way they form the G-matrices, as the values of the $B(E2)$ in ^{12}C change from 5.45 to 6.9 e^2fm^4 for evaluations in a $0\hbar\omega$ and a (complete) no-core $(0 + 2)\hbar\omega$ shell model, respectively. The results, obtained using the OXBASH shell model code [18], are reasonable given that the measured value is 7.77 e^2fm^4. But we note that in other studies [19], made using a standard shell model, problems of only including $2\hbar\omega$ excitations were found. In particular, the neglect of excitations above the $2\hbar\omega$ level forces a much deeper binding energy for the ground state. Addition of the $4\hbar\omega$ excitations, in part, resolved the problem, as has been illustrated in the case of ^{16}O [20].

While a formalism with which the effects of an enumerable $\mathcal{Q}$ space can be accounted may be aesthetically pleasing, it must be remembered at what level of evaluation problems can occur when seeking to apply same to reality. Certainly the approach is built upon a good theoretical base and is an excellent mathematical exercise. But for use in considering real systems, it is not necessarily nor sufficiently complete even at second order. That may be particularly problematic for deformed nuclei. The object of structure and reaction theory is to determine as much information as possible regarding real nuclei and in approaches built upon a Feshbach formalism, all strong coupling features need to be accounted at whatever order they appear. In principle there may no solution to this problem built from theory made using first principles and one may only have the specification of effective forces (phenomenological or otherwise) to enable structure and reactions to be dealt with in any

form of unified way. It would seem that the most fruitful way to proceed is to seek the dominant states in the spaces to which to couple.

---

[1] P. Navrátil and B. R. Barrett, Phys. Rev. C **54**, 2986 (1996).

[2] A. Volya and V. Zelevinsky, Phys. Rev. C **74**, 064314 (2006).

[3] K. Amos, L. Canton, G. Pisent, J. P. Svenne, and D. van der Knijff, Nucl. Phys. **A728**, 65 (2003).

[4] L. Canton, G. Pisent, J. P. Svenne, K. Amos, and S. Karataglidis, Phys. Rev. Lett. **96**, 072502 (2006).

[5] H. Feshbach, Ann. Phys. (N.Y.) **5**, 357 (1958).

[6] H. Feshbach, Ann. Phys. (N.Y.) **19**, 287 (1962).

[7] K. Amos, P. Fraser, S. Karataglidis, D. van der Knijff, J. P. Svenne, L. Canton, and G. Pisent, in *Frontiers in Nuclear Structure, Astrophysics, and Reactions*, edited by S. V. Harissopoulos, P. Demetriou, and R. Julin (AIP, New York, 2006), vol. 831 of *AIP Conf. Proc.*

[8] H. V. von Geramb, K. Amos, R. Sprickman, K. T. Knöpfle, M. Rogge, D. Ingham, and C. Mayer-Böricke, Phys. Rev. C **12**, 1697 (1975).

[9] A. K. Kerman, H. McManus, and R. M. Thaler, Ann. Phys. (N.Y.) **8**, 551 (1959).

[10] K. Amos, P. J. Dortmans, H. V. von Geramb, S. Karataglidis, and J. Raynal, Adv. in Nucl. Phys. **25**, 275 (2000), (and references contained therein).

[11] K. Amos, B. A. Brown, S. Karataglidis, and W. A. Richter, Phys. Rev. Lett. **97**, 032503 (2006).

[12] P. Navrátil and B. R. Barrett, Phys. Rev. C **57**, 3119 (1998).

[13] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. Lett. **84**, 5728 (2000).

[14] A. C. Hayes, P. Navrátil, and J. P. Vary, Phys. Rev. Lett. **91**, 012502 (2003).

[15] S. Karataglidis, P. J. Dortmans, K. Amos, and R. D. Swiniarski, Phys. Rev. C **52**, 861, 3224 (1995).

[16] I. Stetcu, B. R. Barrett, P. Navrátil, and J. P. Vary, Phys. Rev. C **71**, 044325 (2005).

[17] D. C. Zheng, B. R. Barrett, J. P. Vary, W. C. Haxton, and C.-L. Song, Phys. Rev. C **52**, 2488 (1995).

[18] OXBASH-MSU (the Oxford-Buenos-Aries-Michigan State University shell model code). A. Etchegoyen, W.D.M. Rae, and N.S. Godwin (MSU version by B.A. Brown, 1986); B.A. Brown, A. Etchegoyen, and W.D.M. Rae, MSUCL Report Number 524 (1986).

[19] D. J. Milliner, A. C. Hayes, and D. Strottman, Phys. Rev. C **45**, 473 (1992).

[20] W. C. Haxton and C. Johnson, Phys. Rev. Lett. **65**, 1325 (1990).